Benzeneacetic acid, 4-hydroxy-156-38-7 | DTXSID5059745

156-38-7	DIX5ID5059745	

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.72	51.8	0.74	50.3	0.73	52.7	

Model Results

Predicted value: 160 °C

Global applicability domain: Inside

Local applicability domain index: 8.65e-01

Confidence level: 6.25e-01

Nearest Neighbors from the Training Set

Image not found

Benzeneacetic acid, 4-hydroxy-

Measured: 152 Predicted: 160

Image not found

3-Hydroxyphenylacetic acid

Measured: 132 Predicted: 147

Image not found

Benzenepropanoic acid, 4-

hydroxy-

Measured: 131 Predicted: 135

Image not found

3-Hydroxybenzoic acid

Measured: 202 Predicted: 185

Image not found

4-Hydroxybenzoic acid

Measured: 215 Predicted: 187